Lawrence Livermore National Laboratory

Science & Technology Review

December 2011

THE ENERGY SECTOR OF TOMORROW

Also in this issue:

Recording Target Implosions at NIF

A Close Look at Virus Evolution

Software Solutions for Military Analysts

About the Cover

High-performance computing (HPC) is proving to be an important tool in solving the daunting challenges facing the nation's energy sector. As described in the article beginning on p. 4, the HPC resources at Lawrence Livermore provide the computational horsepower needed to study complex scenarios in detail. Working with these simulations, utility companies and resource developers can examine design options without building physical prototypes. In addition, effective use of HPC simulations often reduces the time and cost required to deploy viable technologies. The Laboratory's collaborative projects with the energy sector are demonstrating the competitive advantage HPC offers to help the nation solve environmental challenges, achieve energy independence, and reduce its reliance on imported fossil fuels.

Cover design: Amy E. Henke

About *S&TR*

At Lawrence Livermore National Laboratory, we focus on science and technology research to ensure our nation's security. We also apply that expertise to solve other important national problems in energy, bioscience, and the environment. *Science & Technology Review* is published eight times a year to communicate, to a broad audience, the Laboratory's scientific and technological accomplishments in fulfilling its primary missions. The publication's goal is to help readers understand these accomplishments and appreciate their value to the individual citizen, the nation, and the world.

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Feature

Research Highlights

Departments

Parney Albright Selected as Livermore's 11th Director

Penrose "Parney" C. Albright has been named as director of Lawrence Livermore National Laboratory. Appointed with the concurrence of the Department of Energy (DOE), Albright is the 11th director of the Laboratory since it was established in 1952. He will also serve as president of Lawrence Livermore National Security, LLC (LLNS), which manages the Laboratory for DOE.

"We have selected a leader who brings a fundamental understanding of the importance of science and technology to national and global security," says LLNS chairman Norman Pattiz. "In selecting a leader for Livermore Laboratory, we have found someone who has credibility in the national security arena and a history of addressing a broad range of complex technical issues for the nation's senior leaders.

"Parney understands how the fundamental and applied science, engineering, and computational capabilities of the Lab can contribute to advances in new energy technologies, scientific discoveries, and global security. He has a strong commitment to, and understanding of, the critical role Livermore Laboratory plays in the weapons complex and to the stockpile stewardship program, along with the National Ignition Facility and National Ignition Campaign. His skills and experience will lead the Laboratory into a new era of scientific and technological excellence in service to our nation."

Secretary of Energy Steven Chu adds, "Lawrence Livermore National Laboratory is an integral component of our nation's national security enterprise and one of the Department of Energy's most vital and distinguished laboratories. As we work to accomplish the Department's unique national security missions and make the critical investments required for the future of American innovation, I know we have an outstanding partner in Dr. Albright."

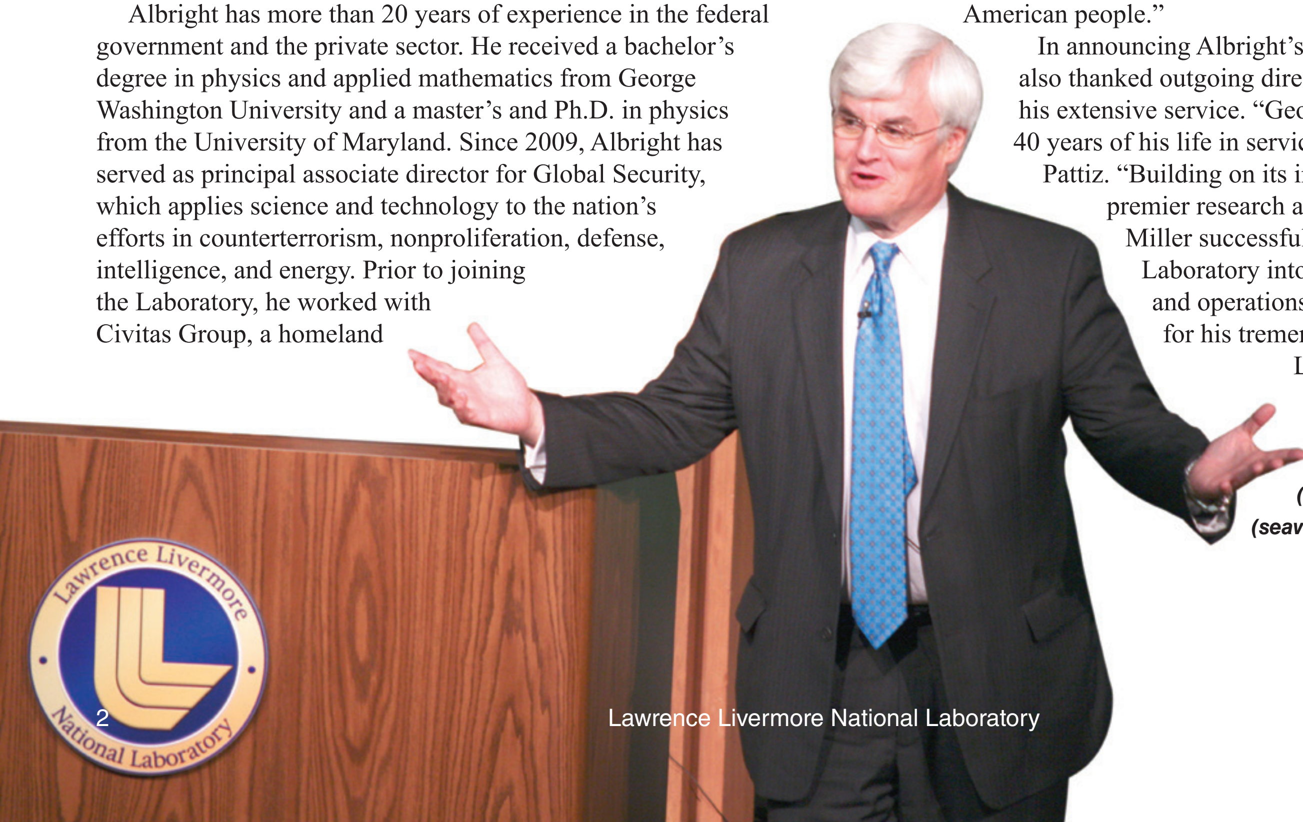
Albright has more than 20 years of experience in the federal government and the private sector. He received a bachelor's degree in physics and applied mathematics from George Washington University and a master's and Ph.D. in physics from the University of Maryland. Since 2009, Albright has served as principal associate director for Global Security, which applies science and technology to the nation's efforts in counterterrorism, nonproliferation, defense, intelligence, and energy. Prior to joining the Laboratory, he worked with Civitas Group, a homeland security consultant in Washington, DC. He has served as assistant secretary in the Department of Homeland Security (DHS); assistant director in the Office of Science and Technology Policy and, concurrently, senior director in the Office of Homeland Security in the White House; and program manager with the Defense Advanced Research Projects Agency.

Albright has extensive experience with interagency and congressional interactions and was a spokesperson for both the White House and DHS to the press and to the broad national research and development enterprise on issues associated with science, technology, and weapons of mass destruction. In addition, he has served for more than 15 years on the staff of the Institute for Defense Analyses, a Department of Defense research and development center, contributing to studies and analyses for senior officials within the Office of the Secretary of Defense on a variety of complex systems and issues at the intersection between technology and policy.

"It is my honor to lead this Laboratory," says Albright. "Livermore Laboratory has a long and rich history of service to the nation. As director, I will work diligently with the help and counsel of the entire Livermore team to ensure this Laboratory remains a preeminent center of excellence in stockpile stewardship; high-energy-density physics; high-performance computing and simulation; and other pillars of world-class science, technology, and engineering—all applied in the nation's interests."

"Having known and worked with Dr. Albright, I look forward to a strong and rewarding partnership," says Thomas D'Agostino, administrator of DOE's National Nuclear Security Administration (NNSA). "As NNSA continues to implement President Obama's nuclear security agenda and make critical investments in the future of our Nuclear Security Enterprise, I know that Livermore will continue to play an important role in the safety and security of the American people."

In announcing Albright's appointment, Pattiz also thanked outgoing director George Miller for his extensive service. "George Miller has given 40 years of his life in service to this nation," says Pattiz. "Building on its incredible history as a premier research and development facility, Miller successfully guided Livermore Laboratory into a new era of science and operations. Our thanks to George for his tremendous commitment; the Laboratory and LLNS will miss his exceptional leadership."



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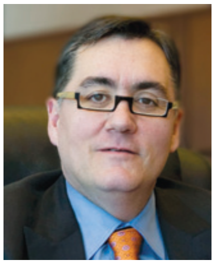
Commentary by Tomás Díaz de la Rubia



High-Performance Computing for Energy Innovation

HIGH-PERFORMANCE computing (HPC) is a proven approach to scientific and technological innovation in which the U.S. enjoys strong international leadership. At the Department of Energy (DOE) national laboratories, HPC has become the "third leg" of research, joining theory and experiment as an equal partner. HPC enables discovery and innovation through the extraordinary simulations it makes possible. These simulations involve hundreds and sometimes thousands of microprocessors working together to mimic physical reality with stunning clarity.

HPC is used increasingly by industry to reduce the time and cost to design, develop, prototype, and deploy new products, materials, and manufacturing processes. As seen in the defense, aerospace, manufacturing, and pharmaceutical industries, this capability brings improved products to market faster and at lower cost. In this respect, HPC provides U.S. industry a competitive edge in the global marketplace.

However, the private sector is not using HPC as aggressively as it could. One U.S. industry in particular—energy—could benefit greatly from leveraging the power of advanced computational techniques to help deliver a more secure and sustainable future. Toward that end, the Laboratory's HPC resources and simulation expertise are helping to advance clean-energy technologies.

As described in the article beginning on p. 4, HPC simulations are the centerpiece of a growing number of Livermore research efforts dedicated to examining in much greater detail the complexities of energy use and generation. For example, to better understand wind power, we are working to model atmospheric turbulence more accurately and determine where to locate wind-turbine farms. Simulations are also helping researchers evaluate several approaches for sequestering carbon dioxide to help mitigate climate change.

We're also using simulations to aid utility companies in designing the electric grid of tomorrow by predicting the availability of intermittent energy sources such as wind and solar power, building more effective defenses against cyberwarfare, and planning for widespread deployment of electric transportation. One new initiative, led by Texas A&M University and sponsored by the DOE Advanced Research Projects Agency–Energy, teams Livermore with other research centers to use HPC to develop a system for real-time, automated control over transmission lines. With such a system, utility operators could optimize electric energy utilization and reduce the number of emergency outages.

The need for energy firms to take greater advantage of HPC was underscored in May 2011, when the Howard Baker Forum, Lawrence Livermore, the Bipartisan Policy Center, and other partners sponsored a National Summit on Advancing Clean Energy Technologies in Washington, DC. The meeting, attended by more than 300 policy makers, energy executives, scientists, and entrepreneurs, featured discussions on promising energy technologies, with a particular focus on exploring how HPC can catalyze rapid advancement of those technologies.

A direct result of this summit was the launching of a pilot program, called the hpc4energy incubator, to spur clean-energy technology innovation through the use of HPC. In October, Lawrence Livermore issued a call for proposals to energy companies to collaborate with us in demonstrating the value of HPC in one of five critical areas: building energy efficiency; carbon capture, utilization, and sequestration; liquid fuels combustion; nuclear energy; and smart grid and power storage. In February 2012, a small set of outstanding proposals will be selected for a one-year pilot in which Livermore researchers and computational scientists will collaborate with industry to more rapidly advance energy technologies.

Initiatives such as the hpc4energy incubator hold the promise of innovative solutions by combining clean-energy technology, the grand challenge of our generation, and HPC, the proven technology accelerator. In the application of HPC modeling and simulation, the capabilities of the DOE national laboratories are unmatched anywhere in the world. The nation has a real competitive advantage in exploiting the power of HPC, and we cannot afford to lose it.

■ Tomás Díaz de la Rubia is deputy director for Science and Technology.

Simulating the Next Generation of Energy Technologies

Livermore's high-performance computing capabilities and expertise in simulation promise to rapidly advance the nation's development of clean-energy technologies.

COMPUTER simulation has become an important tool for finding solutions in almost every field, from physics, astrophysics, meteorology, chemistry, and biology to economics, psychology, and social science. Running simulations allows researchers to explore ideas, gain insights into new technology, and estimate the performance of systems too complex for conventional experimental analysis. For example, automotive engineers perform complex calculations to consider design adjustments before they produce the first physical model. Aerospace engineers use simulations to evaluate proposed combinations of aircraft features instead of building and testing prototype models for each possibility.

Research teams at Lawrence Livermore are now applying the power of high-performance computing (HPC) to improve energy systems throughout the country. Laboratory scientist Julio Friedmann, who leads the carbon-management program for the Global Security Principal Directorate, says, "The energy and environmental challenges facing the nation are so immense, urgent, and complex, high-performance computing is one of the most important tools we have to accelerate the development and deployment of solutions. Simulations will give us the confidence to move ahead more rapidly, and we don't have the luxury of learning the slow way."

HPC will provide U.S. industry with a competitive advantage in solving environmental challenges, achieving energy independence, and reducing the nation's reliance on imported fossil fuels. In addition, using these computational tools to explore technology solutions will save time and money by helping utility companies reduce capital expenditures, avoid industrial failures, and prevent damage to power-generation equipment.

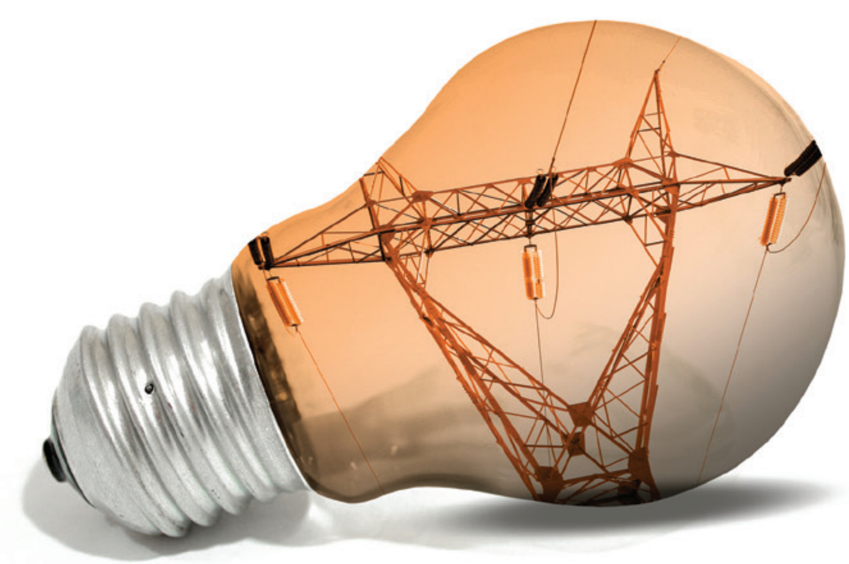
A Foundry for Solutions

According to Friedmann, partnerships between national laboratories and private industries are advancing the use of simulation to evaluate new concepts for power generation and efficient energy use. Traditionally, technology development for energy utilities and other industries starts with producing a benchtop model. When a new design proves successful, the benchtop is scaled up in power and capacity, with each subsequent model taking about two years to produce.

With HPC, design engineers can scale through simulated prototypes much more quickly. "HPC allows us to skip steps in the scaling process," Friedmann says. "Without these simulations, we'd have to keep building larger prototypes from a benchtop to a 10-kilowatt model on up to 100 kilowatts, 1 megawatt, and so forth."

In support of stockpile stewardship, the Laboratory has already created many complex simulation tools and developed the expertise to run them effectively on massively parallel computer systems. The successful application of HPC to help maintain a reliable nuclear weapons stockpile has increased confidence in the power and effectiveness of these tools. As a result, large and small firms throughout the energy industry are interested in tapping into the Laboratory's HPC resources.

"Utilities and those involved with improving energy efficiency work with computational tools every day," says John Grosh, deputy associate director for Computation's programs. "They are frequently hampered, though, because they are running applications on desktop computers or small server systems. The computational horsepower offered by our machines is 1,000 to 100,000 times



greater than what they have available." HPC simulations can examine complex scenarios with fine resolution and high fidelity—that is, with the level of detail and accuracy required to ensure that simulated results emulate reality.

In looking for partnership opportunities that are most suitable for addressing national problems, Friedmann has found many energy projects in which HPC simulations could play an important primary or supporting role, improving the quality of solutions and the rate of deployment. He notes, however, that simulation and modeling are not the goal. "They are the medium by which we deliver solutions to problems," he says. "Like a foundry, we want to forge solutions to address threats to American competitiveness and energy security."

These challenges are providing a wide range of opportunities where HPC simulations can make a difference. One Laboratory effort is focused on predicting how the intermittent nature of renewable energy sources such as wind and solar power will affect electricity generation. In another project, Livermore researchers are developing HPC simulations to evaluate the environmental implications of new technologies such as those for enhanced energy production and carbon capture and sequestration. Says Friedmann, "Delivering solutions to these problems is our measure of success."

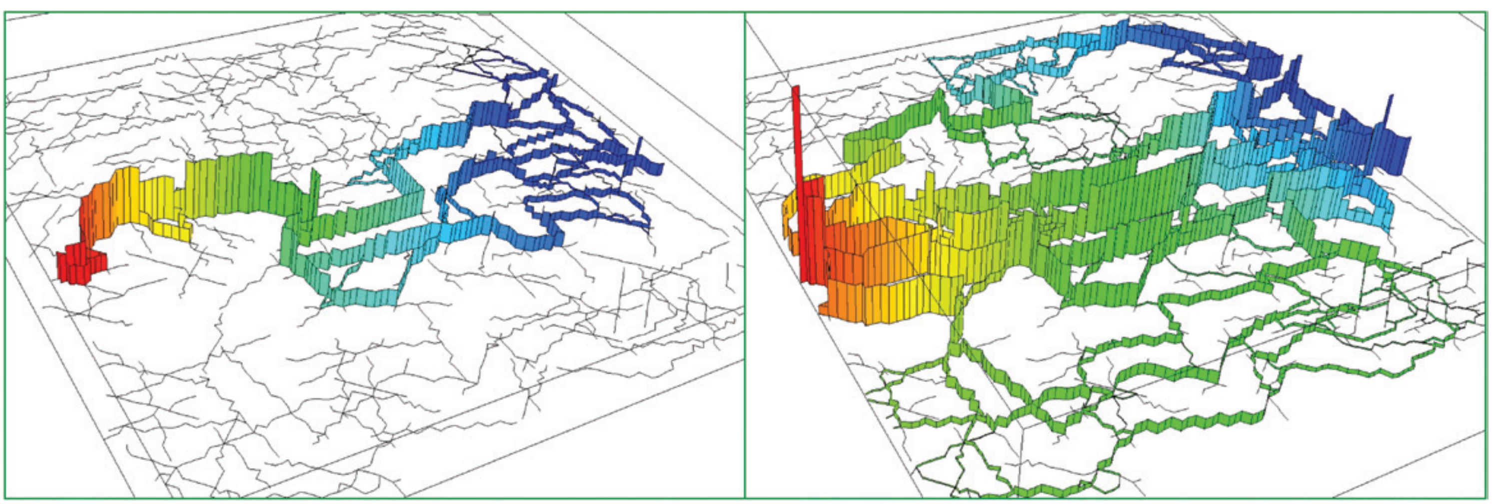
A New Look at Today's Technology

Improving the nation's energy security is not only about developing advanced technologies. It also involves improving how available resources are used today. Livermore geophysicist Rick Ryerson in the Physical and Life Sciences Directorate is leading one such effort: applying HPC calculations to predict how best to create subsurface fracture networks for enhanced recovery of shale gas and geothermal energy.

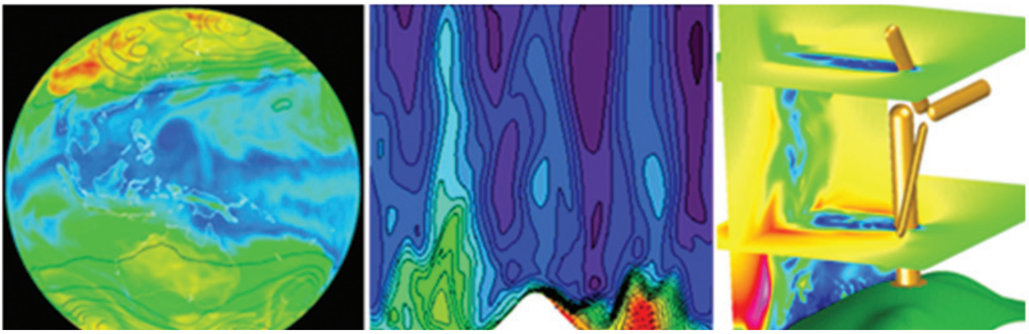
"Before we induce hydraulic fracturing or stimulate gas flow in an underground network, we need to evaluate the effects of our proposed techniques," says Ryerson. "Then we can refine the best methods to get improved energy extraction in a safe and environmentally responsible manner."

Jeff Roberts, who leads Livermore's Renewable Energy Program, notes that this multidisciplinary effort builds on the Laboratory's expertise in seismology and rock mechanics as well as HPC. "Our existing codes were not designed to simulate fracture generation in tightly coupled geologic materials—for example, areas where underground water flows through different rock layers," says Roberts. "A key challenge in resolving this issue has been to develop a simulation framework that allows us to explore the interactions between fluids and solids during the fracturing process."

Livermore researchers are also part of the Greater Philadelphia Innovation Cluster (GPIC), a collaboration designed to help organizations build, retrofit, and operate facilities for greater energy efficiency. "We need better insight into how buildings consume energy and lose heat," says Grosh. "Simulation tools can help us gain this understanding at higher fidelity." With that information, engineers, architects, and operators can modify designs to improve a facility's energy efficiency.



High-performance computing (HPC) simulations by Pengcheng Fu, a postdoctoral researcher at Livermore, predict the increased flow of, for example, shale gas or geothermal energy when an underground reservoir is stimulated with fluid overpressure. The results shown here compare the fracture network in a 100- by 100-meter reservoir before (left) and after (right) stimulation. Bar heights indicate flow rate. Color represents fluid pressure, which is highest (red) at the injection well and lower (blue) at the production well. Stimulated flow engages fractures in the lower regions of the network, allowing developers to extract energy from this part of the production field.



Finer mesh grids applied over a zone of interest improve the numerical resolution of HPC simulations. This example shows the cascade of scale provided by a nested grid resolution, allowing researchers to examine in detail how global circulation patterns (left), local terrain (middle), and placement of individual wind turbines (right) might affect wind currents.

As part of this project, Laboratory researchers are developing algorithms and other computational tools to quantify the uncertainties in the energy simulations they are running. Uncertainty quantification is a growing field of science that focuses on quantifying the accuracy of simulated results, in particular, which predicted outcomes are most likely to occur. (See *S&TR*, July/August 2010, pp. 12–14.) Determining the quantitative level of model accuracy is especially difficult because calculations include approximations for some physical processes and not all features of a system can be exactly known. By quantifying the uncertainty and numerical errors in simulations of a facility's energy consumption, Livermore researchers and their GPIC partners can develop more robust and effective building controls.

Forecasts in the Wind

One of the more difficult problems facing utility companies is predicting the availability of intermittent energy sources such as wind and solar power. A Livermore team led by Wayne Miller in the Engineering Directorate is refining HPC simulations of wind energy to improve forecasting accuracy. For this effort, the team has modified the Weather Research and Forecasting (WRF) code, a public-domain code designed to model weather patterns over a segment of the globe, such as the entire state of California. "WRF detects large-scale weather motions and simulates patterns over thousands of square kilometers," says Miller. "For example, it can pick up the large cyclonic low-pressure systems that come down the California coast. But that representation is too coarse to capture accurate forecasts in a particular spot, such as at a wind farm in the Altamont Hills east of Livermore."

To improve the numerical resolution of the simulated results, the team applies finer mesh grids over the zone of interest, a process called nesting. By nesting the grid resolution, researchers can see in detail how changes in global circulation patterns and local terrain affect the thermal cycling that drives winds on a daily schedule. Postdoctoral scholar Katie Lundquist is working to incorporate the Immersed Boundary Method into the base WRF code. This model will more precisely represent complex terrain, such as mountains, foothills, and other topographic changes that WRF does not resolve, and thus improve the accuracy of the simulated results.

Miller's team is also developing computational tools to model atmospheric turbulence. Gusts are a form of turbulence that can significantly alter the availability of wind energy at a site as well as the stability and uniformity of wind currents—characteristics that can affect a power plant's production capabilities. In addition, says Miller, "A wind gust strong enough to heel a sailboat over can be trouble for a turbine," causing component fatigue or even failure ahead of a turbine's rated lifetime.

In-depth analysis of wind patterns provides valuable information for determining where to locate large wind-turbine farms. Building a wind farm requires considerable capital expenditures, and choosing a site can affect a developer's return on investment. HPC simulations can incorporate field data as well as historical averages of wind patterns to characterize potential locations and predict the amount of power each one could produce.

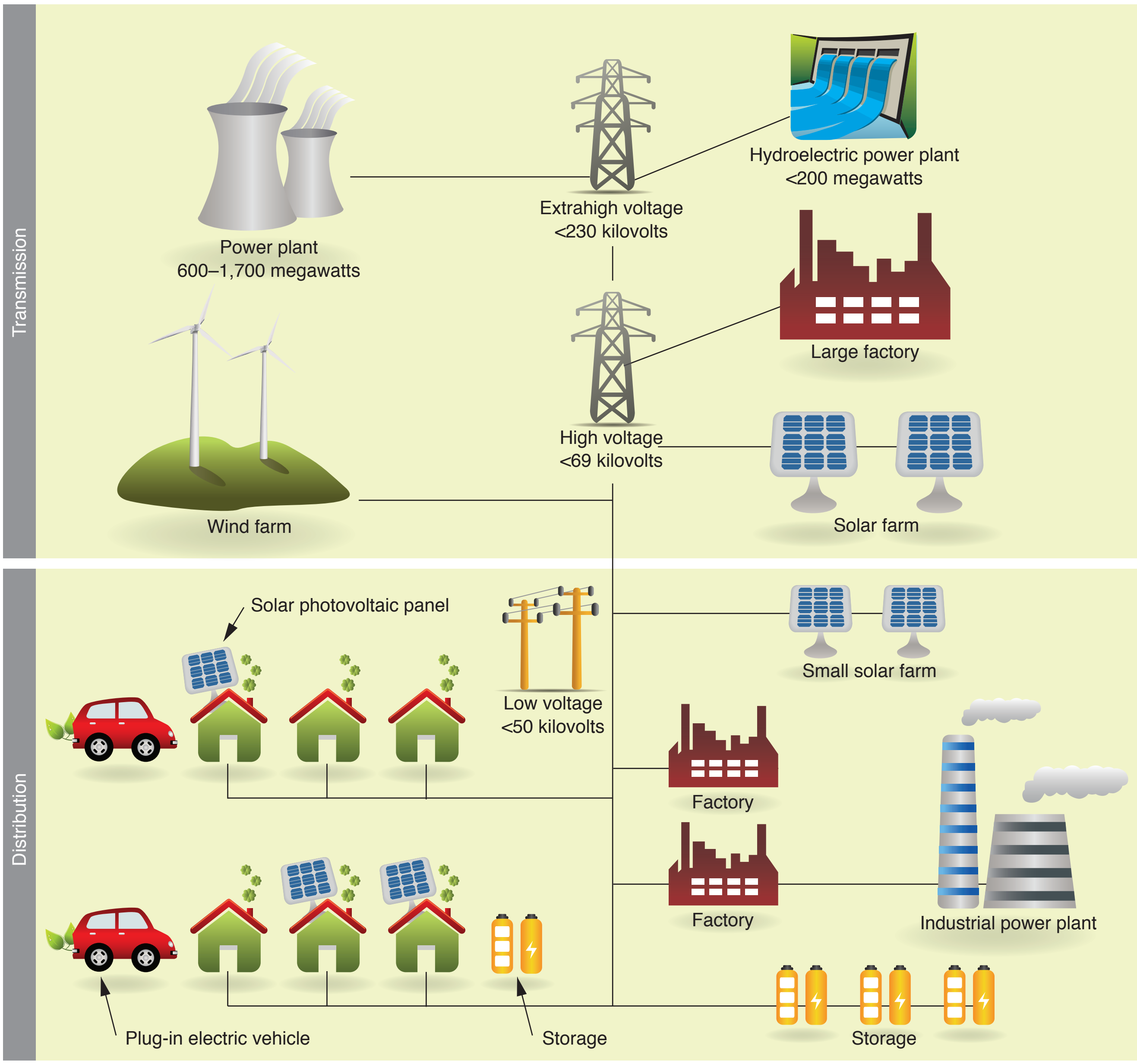
Livermore simulations will also evaluate how wind forecasts for an area can predict energy production at a particular wind farm, information utility companies can use to fine-tune the balance between supply and demand. Many utilities supplement peak load requirements with gas turbines to ensure that the amount of power supplied to the grid remains steady even as wind patterns change. When demand for power peaks, as it would on a hot, still day when many people turn on their air conditioners, gas turbines generate the peak energy needed to help meet those demands. At other times, wind alone can generate the power required.

With timely, accurate predictions of these changing conditions, utilities could make adjustments more quickly and better control their operating costs. The simulations developed to date do not run in real time, but researchers at Livermore and elsewhere are refining the models to operate faster.

Prior to supercomputers, the energy industry relied on experimental data and observations, both of which are expensive to acquire. Researchers must gather enough samples to guarantee that results are statistically valid. As an example, Miller describes an effort to collect data on offshore wind power. The average cost for an offshore meteorological tower is $5 million, and surveying the entire length of the California coast would require 1,000 towers. "Computer simulations are wildly cheaper than that project would be," says Miller. He notes that field samples are still necessary, providing data to validate model accuracy. "If a simulation starts to diverge from reality, we can use field data to tune the model into alignment, even as it's running."

Putting Carbon in Its Place

New technologies to capture carbon dioxide before it reaches the atmosphere are also benefiting from HPC simulations. Livermore researchers have evaluated several approaches for sequestering this greenhouse gas as part of the efforts to mitigate climate change. (See *S&TR*, December 2010, pp. 22–24; May 2005, pp. 12–19.) An innovative project led by computational biologist Felice Lightstone



This conceptual drawing illustrates the vast, complex resources in the electric grid of tomorrow. Livermore's expertise in HPC is advancing the development of new technologies to secure the nation's energy supply for years to come.

is using HPC simulations to design a synthetic lung enzyme that can catalyze the capture process before carbon is released to the atmosphere by coal-fired power plants. (See *S&TR*, March 2011, pp. 4–9.)

To design the catalyst, Lightstone's team is borrowing methodologies from the pharmaceutical industry. In searching for an effective, broad-spectrum antibiotic, drug developers must identify key interactions between small molecules that bind to specific proteins. Designing the synthetic lung catalyst involves making and breaking chemical bonds as well. HPC tools allow the team to quickly analyze candidate compounds. "Our goal is to give the experimentalists a lot of suggestions for effective molecular combinations," says Lightstone. "Then we provide a fast, iterative feedback loop to modify the options."

Without HPC, the turnaround time would make this work impractical. "We'd have to do it the old-fashioned way—think of an idea and try it in the lab," says Lightstone. If researchers relied only on trial and error, they would have to synthesize samples of each candidate molecule to be tested, a difficult and time-consuming process. Instead, using HPC simulations, they can design hundreds of possible combinations and synthesize only the most promising candidates. After creating the catalyst, the researchers will hand it off to Babcock and Wilcox, an international provider of energy products and services, for small-scale systems testing.

Roberts adds that HPC is also important for evaluating the effects of carbon sequestration technologies. "We need to improve our understanding of fluid flow in underground reservoirs," he says. "For example, where does carbon dioxide go when it's pumped into the subsurface? And how does that fluid movement affect the surrounding geologic layers." Evaluating new technologies for carbon capture and sequestration is a long-term, complex process, but HPC simulations speed up the process significantly. Says Friedmann, "With simulations, we expect to cut the deployment cycle in half, reducing a 10- or 15-year timeline to only 5."

A Thousand Scenarios in a Day

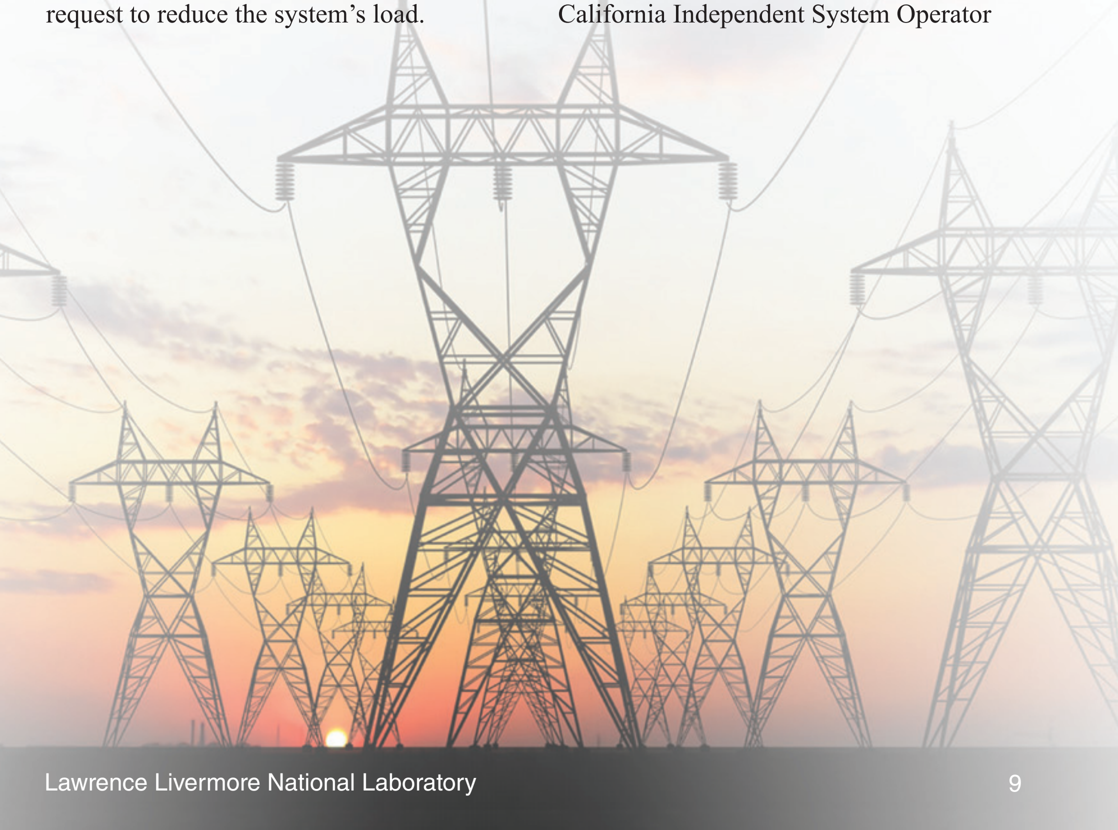
Energy networks are vast and complex. A typical distribution system of a trunk power line may have 2,000 circuits. California has 20,000 distribution systems, with millions of power lines lacing the state. Millions of variables must be examined to understand the system as a whole and recommend improvements, a job best suited to supercomputers.

To help utility companies determine what resources are needed for the electric grid of tomorrow, Livermore scientists are using HPC simulations to model the impacts when generation capacity is increased by adding a large number of intermittent wind and solar resources to the grid. Instead of building conventional generating capacity to back up these intermittent resources, grid operators could rely on techniques such as distributed energy storage or demand response, in which consumers shut off appliances on request to reduce the system's load.

"The advent of distributed storage, generation, and demand response has increased the number of grid state and control variables by orders of magnitude," says Livermore scientist Thomas Edmunds, who works in the Engineering Directorate. "We need larger-scale planning and operations models to optimize the performance of these systems." A Laboratory Directed Research and Development project led by Edmunds is focused on developing optimization algorithms for this application.

He notes that HPC can also contribute to grid reliability. Grid managers must operate the system in a fault-tolerate mode with generating levels set such that no single failure will cause a widespread blackout. To ensure reliability, researchers must analyze many independent models of the grid with different failure modes. "This problem is ideal for high-performance computing," says Edmunds.

Legislation enacted in California calls for 33 percent of the state's energy supply to come from renewable resources by 2020. Mathematician Carol Meyers of the Engineering Directorate is working on a study initiated by the California Public Utilities Commission and managed by the California Independent System Operator

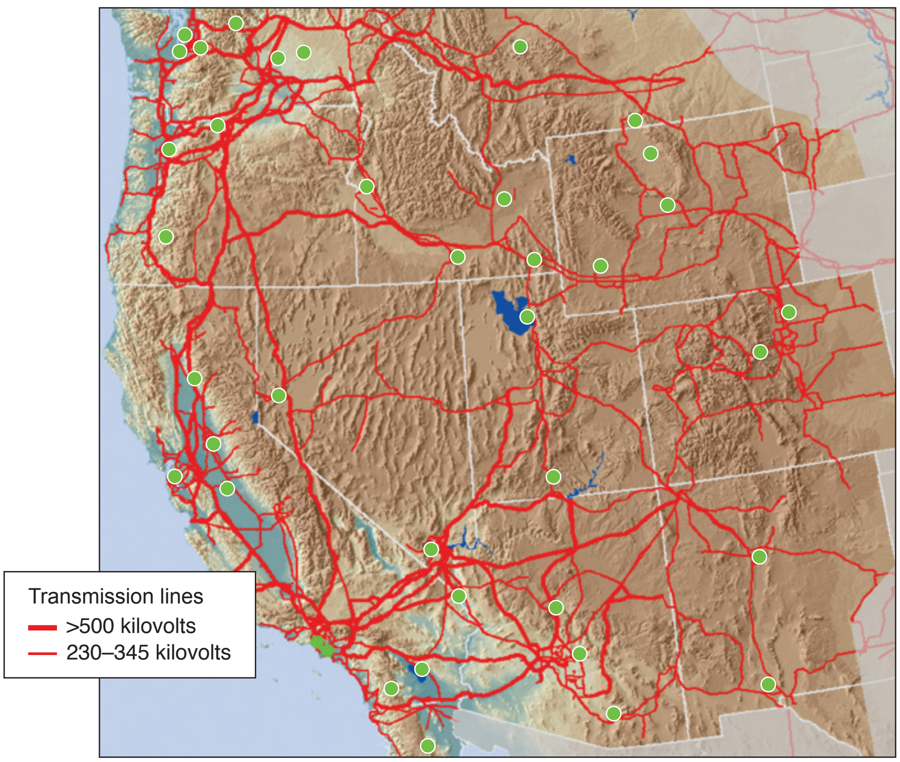


(CAISO) to help determine how the 2020 standard will affect operations of the state's grid. "Potentially billions of dollars are at stake in terms of backup generation and transmission costs to incorporate renewable resources on a large scale," says Meyers. "The power utilities need to better understand all of the issues involved so they can adapt to distributed generation."

For the CAISO study, Meyers and software developers at Energy Exemplar adapted the company's PLEXOS energy simulator to run on the Laboratory's supercomputers. "PLEXOS is front-end software that generates the mathematical model for our simulations," says Meyers. In demonstration runs on the Hyperion test bed, PLEXOS looked at the 2,100 generators across the entire western grid, plus a large number of load, storage, transmission, and reserve requirements. The resulting model included more than 225,000 variables and 400,000 constraints and took an incredibly long time to run—several days to compute one yearlong scenario.

"We dug into the model to determine what slowed it down," says Meyers. The bottleneck was in the Mixed Integer Programming solver, which takes a mathematical description of the variables, constraints, and objective function and solves the model. "IBM provided licenses for CPLEX, their state-of-the-art mixed-integer optimization software," she says. Adding CPLEX allowed the researchers to run simulations in parallel. When combined with the Laboratory's HPC processing power, the modified PLEXOS could simulate a thousand scenarios a day. The development team then modified the mathematics routines behind the model to improve variable interactions. The resulting calculations ran four times faster.

"HPC has the potential to be game-changing in the energy industry," says Meyers. "It not only answers existing questions but also expands the very nature of questions to be asked." The team's future work involves streamlining the PLEXOS–HPC user interface, modifying the optimization routines, and collaborating with IBM to extend CPLEX to run on massively parallel systems. The work has already proven valuable, serving as the demonstration test case for a proposal to simulate the possible consequences of end-to-end changes to the energy system.

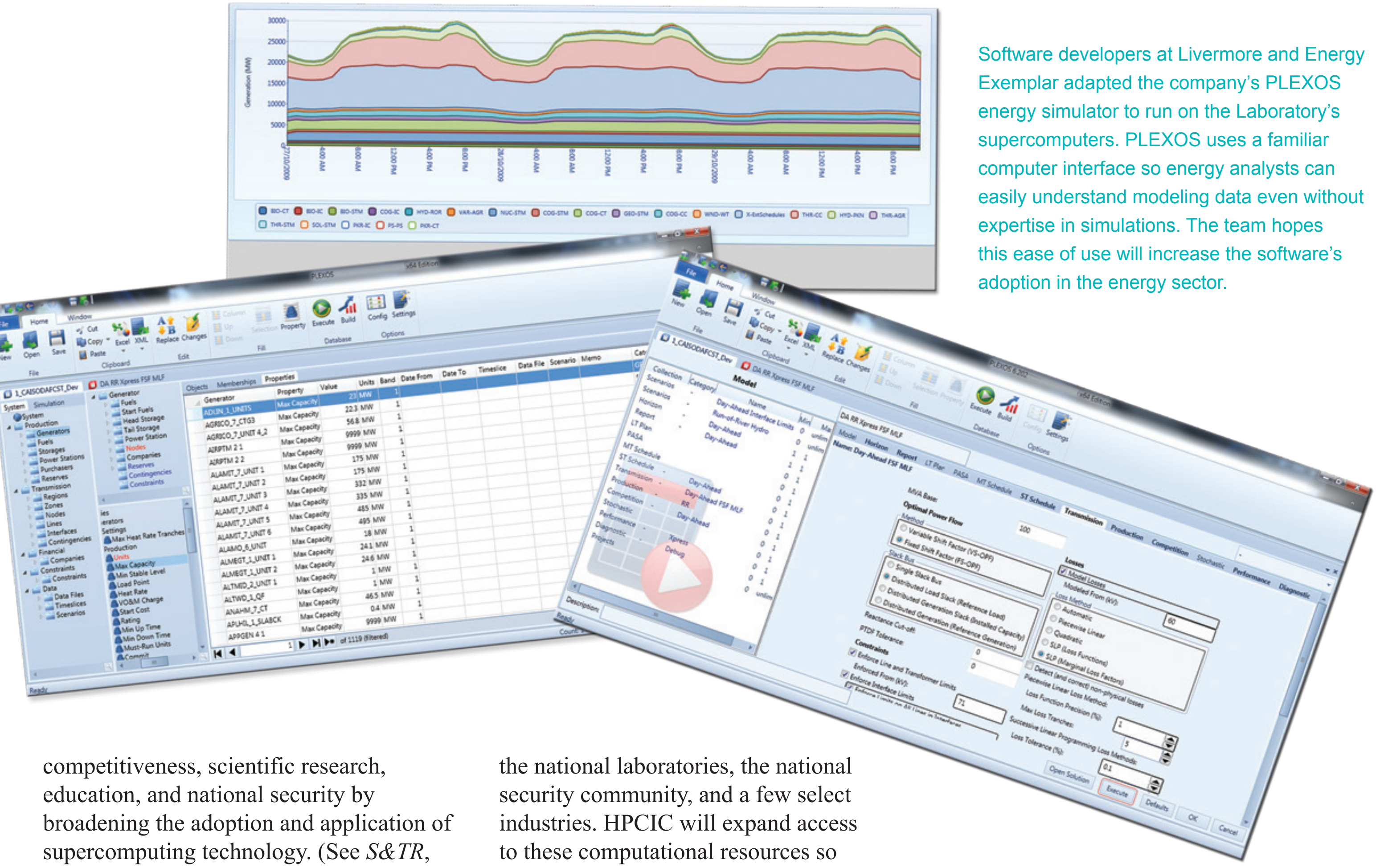


This map shows the electricity transmission lines (red lines) and the load or generation centers (green dots) for the western U.S. Simulations of these electric grid resources produce massive amounts of data.

Reduced Barriers to Partnership

Once progress has been made in these projects, the Laboratory and other entities will reach out to large and small companies that cannot afford to invest in HPC resources themselves. Giving potential partners an opportunity to probe the world of HPC simulations allows them to see which tools might be adapted to meet their needs. According to Friedmann, Livermore's plan is to develop a Web portal that provides links to available tools and promotes those resources to potential collaborators at universities and industry.

The new High-Performance Computing Innovation Center (HPCIC) is also helping to extend the Laboratory's HPC capabilities to energy-related work. Part of the Livermore Valley Open Campus adjacent to Lawrence Livermore and Sandia national laboratories, HPCIC is a public–private partnership whose mission is to boost American industrial



Software developers at Livermore and Energy Exemplar adapted the company's PLEXOS energy simulator to run on the Laboratory's supercomputers. PLEXOS uses a familiar computer interface so energy analysts can easily understand modeling data even without expertise in simulations. The team hopes this ease of use will increase the software's adoption in the energy sector.

competitiveness, scientific research, education, and national security by broadening the adoption and application of supercomputing technology. (See *S&TR*, March 2011, pp. 22–25.) The center provides partnering organizations with access to secure supercomputer resources and computational expertise that would otherwise be unavailable.

HPCIC projects will focus on big, complex challenges and opportunities in the energy sector as well as in climate science, health care, manufacturing, and bioscience. The center will allow industrial partners to access the full range of scientific, algorithmic, and application support available at the national laboratories. Grosh notes that although many companies develop codes that run on desktop computers, the ability to write for modest to large computing systems is much rarer outside the national laboratories, the national security community, and a few select industries. HPCIC will expand access to these computational resources so that industrial partners can perform virtual prototyping and testing, conduct multidisciplinary science research, optimize software applications, and develop system architecture for next-generation computers. "With this new capability, we foresee transforming the way U.S. industry uses HPC and providing an innovation advantage to the energy sector," says Grosh.

Friedmann adds, "Supercomputing centers are popping up around the country, and they're all looking for applications in manufacturing and energy and for software that is ready to run on their machines. Working with them to apply our expertise in HPC is a natural outgrowth of the Laboratory's mission. We have an opportunity to merge diverse projects into a coherent effort and create a knowledge pipeline for tackling important national issues. The growth potential for the Laboratory is immense."

—Kris Fury

Key Words: carbon capture and sequestration, clean energy, energy sector, high-performance computing (HPC) simulation, High-Performance Computing Innovation Center (HPCIC), smart electric grid, wind energy.

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ARC Comes into Focus

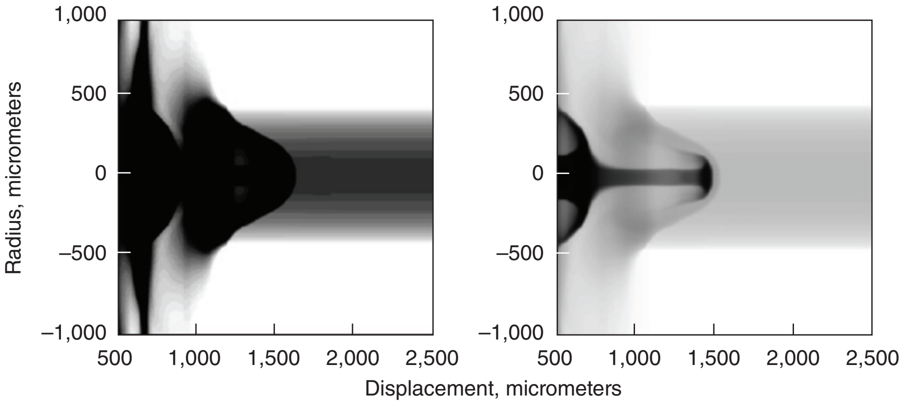
THE time it takes to complete a shot on the National Ignition Facility (NIF) at Lawrence Livermore makes the blink of an eye seem almost like an eternity. From the moment the initial laser burst is created to the completion of a typical high-energy-density science experiment, less than two-millionths of a second elapse. In the process, NIF's 192 beams deliver energy in the form of laser light that heats a target to temperatures of tens of millions of degrees and compresses it to pressures many billion times greater than Earth's atmosphere. Obtaining meaningful information about the physical processes occurring in the tiny target over timescales measured in picoseconds (trillionths of a second) has required researchers to develop a new generation of ultrafast, ultrahigh-resolution diagnostic devices. (See *S&TR*, December 2010, pp. 12–18.)

A new tool called the Advanced Radiographic Capability (ARC) will soon provide a unique capability in NIF's arsenal of detectors, spectrometers, interferometers, streak cameras, and other diagnostic instruments. ARC is a petawatt-class laser—that is, its peak power exceeds a quadrillion (10^{15}) watts—and is designed to produce brighter, more penetrating, higher energy x rays than is possible with conventional radiographic techniques. Says Greg Tietbohl, ARC project manager, "ARC allows us to see through the dense core of fuel in a target as it is being compressed."

With ARC, scientists can record a series of snapshots revealing the dynamics of materials under extreme conditions of temperature and pressure. When combined, these images will reveal changes in complex two-dimensional features over time.

Single-frame radiography using x-ray backlighters is already deployed at NIF, but this capability lacks the image quality, penetration levels, speed, flexibility, and multiframe functionality of the ARC design. ARC splits each of four NIF beams into two apertures, producing up to eight petawatt-class laser pulses that can be used to create high-energy x-ray images of the target. Each of these split beams can be adjusted independently with energy ranging from 0.4 to 1.7 kilojoules, pulse duration between 1 and 50 picoseconds, and delay up to 80 nanoseconds. "In a single beam, ARC will deliver up to 500 trillion watts (terawatts) of power—the same level of power NIF generates with 192 beams,"

Livermore's novel "folded" compressor vessel design dramatically reduces the footprint of the Advanced Radiographic Capability (ARC). Shown here is ARC project manager Greg Tietbohl next to one of the system's two compact vessels, which together hold eight compressors.



ARC allows scientists to peer inside extremely dense objects during National Ignition Facility (NIF) experiments. Simulated images illustrate how current radiographic capabilities (left) may be improved using ARC-generated x rays (right). (Courtesy of Keith Matzen, Sandia National Laboratories.)

says Constantin Haefner, the lead scientist for the ARC team. This power and flexibility put ARC in a league of its own.

Hitching a Ride on NIF

Work on the ARC concept began in 2002 as a Laboratory Directed Research and Development (LDRD) project led by Livermore scientists Chris Barty, Mike Key, and John Caird. The project's goals were to create innovative technologies that could produce petawatt pulses from modified, individual NIF beamlines and adapt them for radiographic and high-energy-density applications. Of particular interest was the possibility of using petawatt-class pulses on NIF to create the ultrashort, high-energy x rays required for x-ray radiography of laser fusion ignition and implosion experiments.

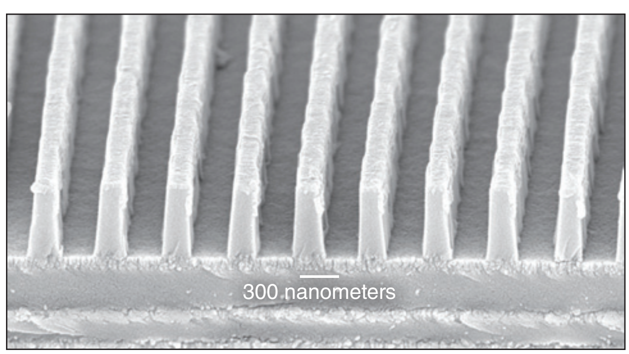
In 1996, Livermore researchers demonstrated petawatt laser pulses for the first time. Those experiments, which used a modified beam of the Nova laser system, revealed that the high-intensity laser interactions were significantly more efficient in generating high-energy x rays. (See *S&TR*, September 1995, pp. 24–33; December 1996, pp. 4–11.) Predictions based on the Nova petawatt experiments and later experiments at other facilities suggested that one-half of only one NIF beam (a split beam) could produce the necessary high-energy x rays. Achieving the same results with the existing NIF setup would require focusing more than 60 of the regular long-pulse beams onto one x-ray generation target.

ARC reaches the extreme laser intensities through chirped-pulse amplification, a common architecture for short-pulse lasers. In this process, an ultrashort laser pulse, only picoseconds or femtoseconds (10^{-12} to 10^{-15} seconds) long, is first stretched in time to reduce its intensity. The pulse's frequency content is distributed in time to create a nanosecond-long (10^{-9} second), frequency-swept (chirped) pulse that can be safely amplified without generating intensities above the damage limit of laser glass and optics. After amplification, the chirped pulse is passed through an arrangement of diffraction gratings (pulse compressor) to undo the frequency sweep and re-create the initial short pulse, thus producing a high-energy, high-power laser pulse.

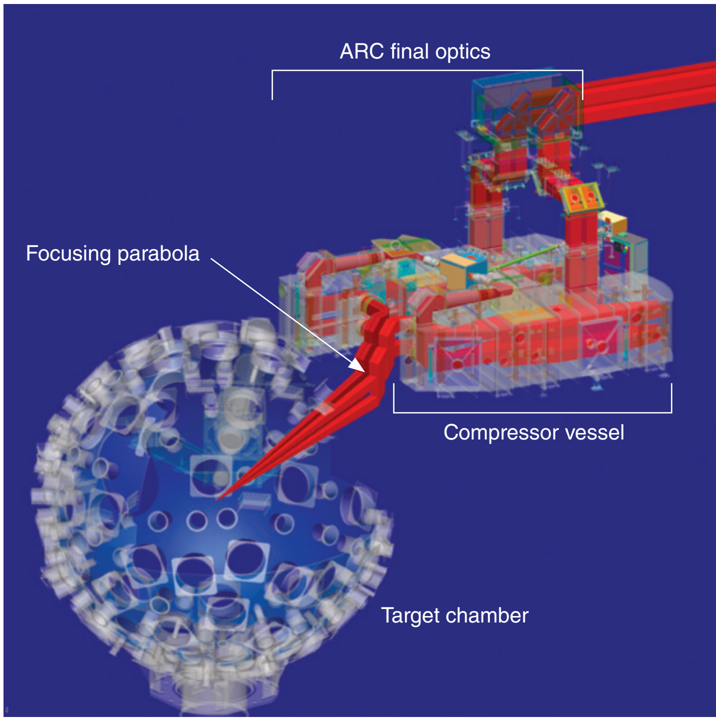
Implementing chirped-pulse amplification on NIF presented numerous challenges and required several new technologies and techniques. For example, pulse compression gratings had to be fabricated of sufficient size, efficiency, and damage resistance to handle the record-setting beam energy produced by NIF. Pulse compressors were redesigned to be 10 times more compact to be compatible with the existing NIF building and layout, and the seed laser systems were modified to be robust yet compact enough to fit into the existing NIF architecture. Techniques were also developed to capture the full characteristics of the ARC laser pulse in one shot and to allow rapid switching of designated NIF beams from long- to short-pulse operation and back.

Miles of Grooves

Prior to 2002, Livermore was already producing the world's largest diffraction gratings: 96-centimeter-wide gold gratings that were used to produce the 500-joule, petawatt pulses on Nova. However, these gratings were not large enough to handle the increased beamline energy produced by NIF. To resolve this issue, optics engineer Jerry Britten and his colleagues worked on an



This scanning electron micrograph shows the surface detail of a dielectric grating. By precisely controlling the width and height of surface grooves, Livermore researchers can produce diffraction gratings with efficiencies close to the theoretical limit and the highest possible damage threshold.



With the folded compressor design and a new laser beam centering and pointing system, ARC is compact enough to fit inside the existing architecture of NIF's 30-meter-diameter target chamber.

LDRD-funded project to develop a new multilayer dielectric grating technology and the related tools for manufacturing the required 1-meter-wide compression gratings. The new gratings allow the laser energy density to be increased by 10 times at significantly higher efficiency.

Britten notes that designing the ion-beam etcher, which he likens to a sandblasting tool for ions, was a crucial step in producing gratings that meet ARC's requirements. In particular, careful control of the width and height of surface grooves in the dielectric film is the key to obtaining efficient diffraction with the highest possible damage threshold. An astonishing 450 miles (730 kilometers) of lines cover the surface of one grating. Developing measurement techniques to confirm surface and groove uniformity together with cleaning techniques to maintain an extremely low level of surface contamination was also essential for obtaining optimum grating performance. (See *S&TR*, September 1995, pp. 24–33.) Tests at ARC's precision damage test facility have confirmed that ARC dielectric gratings are the highest damage threshold gratings of their type yet fabricated.

Space Constraints Spur Ingenuity

Grating development was not the only difficulty to overcome. Because the ARC design came together after NIF was designed and largely built, the project team faced the fundamental challenge of fitting the system in and around the giant NIF laser. Accommodating the compressors in the limited floor space near the target chamber was particularly difficult. Even with dielectric gratings placed at a high incident angle, the laser pulse compressor would be the size of a railroad car, which is more than 17 meters long. The ARC design required compressor vessels to be less than 8.5 meters long.

The answer was to "fold" the compressor to make it more compact. In the resulting design, four pairs of optical gratings are arranged on two levels, in two compressor vacuum vessels. Each split beam hits four gratings as it travels. A curved telescope mirror (parabola) focuses the set of four beams, and a mirror aims them at the specific targets. "We have developed the smallest compressor in the world for this type of laser," says Haefner. The optical gratings are designed with two groove densities, allowing them to be placed close to one another and greatly reducing the overall footprint of the compressor arrangement.

The compressor design, however, left no space for standard alignment techniques. As a result, the ARC team developed a new laser beam centering and pointing system to ensure that each ARC beam is pointed and focused precisely. Designed by Livermore optical engineer Mike Rushford to meet space constraints in the ARC vessels, the compact and reliable system won a 2009 R&D 100 Award. (See *S&TR*, October/November 2009, pp. 18–19.) As Haefner notes, "We have a nonstandard compressor and no room for standard alignment techniques, so we had to come up with nonstandard techniques." The system uses one lens and camera, rather than the standard two, for image pointing and centering information. The single camera registers where the beam came from (for centering) and where it is going (for pointing) at precisions within 10-thousandths of a degree.

Integrating Performance

Modeling, assembling, testing, and diagnosing ARC subsystems and integrating performance results have been crucial to ARC development and systems qualification. Though a diagnostic itself, ARC is complex enough to require its own diagnostic tools.

Short-pulse, high-intensity laser light is extremely difficult to measure because it is very short in time and its characteristics change when it travels through material such as lenses and glass windows. Furthermore, measuring the pulse duration would require an electrical sensor 10,000 times faster than those currently available. Instead, ARC scientists are using the laser to measure itself. The technique they use, frequency-resolved optical gating, redirects a "slice" of the laser pulse from the ARC beam through a nonlinear crystal and into a spectrometer. The sample slice provides information about ARC's pulse shape and characteristics.

ARC's test facilities provide data to input into and compare against models for predicting the system's overall performance.

In 2009, the Livermore researchers assembled a scaled-down compressor at the output of a preamplifier module in an off-line facility to measure the performance of the full ARC injection laser system (fiber front end plus preamplifier module) as well as several key diagnostics. John Crane, the ARC systems engineer, says, "It is important to assemble the subsystems and measure how they perform together." Results from these experiments led the team to replace the large fiber amplifiers with spectrally agile, dual regenerative amplifiers. The new injection system produces 50 times the energy of the original ARC design.

Testing also confirmed that the ARC front end can produce more than 1 terawatt of peak power. In addition, the researchers verified that a technique they developed accurately measures the amount of pulse stretch and compression. In contrast to nonlinear techniques, the new approach allows them to precisely predict and optimize ARC's power performance without firing a single pulse. "Proving this technology works was a major achievement," says Haefner. "Optimizing the short-pulse performance typically takes tens to hundreds of iterations."

Illuminating a Range of Experiments

ARC's key application, of course, will be to image, using backlighting, the time evolution of targets illuminated by NIF beams at the center of the target chamber. For backlighting, up to eight wires, each 30 micrometers in diameter, can be placed around a target to convert ARC's ultraviolet light into a burst of x rays. The wire acts as an x-ray point source, illuminating the target, while gated imaging cameras capture an image. Each camera has a scintillator plate that lights up when x rays hit, generating visible light that can be recorded by a regular camera. The wires are arranged at different points in space and can be hit by the ARC beams delayed in time to enable high-energy x-ray radiographic capability with both multiple time frames and multiple views. Compared with the picosecond pulses produced by ARC, the camera is quite slow, so it records all the data points at once.

ARC lead scientist Constantin Haefner is developing diagnostics for the petawatt-class laser system. These diagnostics were used in tests of an ARC prototype that produced an extraordinary 1 terawatt of power out of just the front-end system.

Beyond backlighting, ARC applications are surprisingly varied and numerous. Livermore physicist Hye-Sook Park studies materials under high pressure (see *S&TR*, January/February 2007, pp. 4–11) and is one of many experimentalists eager for ARC to come online. Working with the short-pulse capability provided by OMEGA EP at the University of Rochester's Laboratory for Laser Energetics, Park has produced high-quality radiographic data for high-energy-density experiments on tantalum. Unfortunately, she has reached the limit of conditions OMEGA can produce. This stockpile stewardship research requires pressures up to several hundred billion pascals, and for that, says Park, "We need both NIF and ARC. NIF is the only laser that can achieve such high pressures, and ARC is essential for probing materials under those conditions."

ARC is also ideal for experiments on a state of matter found only in gamma-ray bursts, black holes, active galaxies, and the universe shortly after the big bang. Physicist Hui Chen works with a team of Livermore researchers who are using lasers to generate and study positrons. These experiments require the unique capabilities of high-power, short-pulse lasers to produce a tightly focused "photon bullet," as Chen describes it, about 0.01 millimeters across and 0.3 to 3 millimeters long packed with trillions of trillions (10^{24}) of photons. By concentrating the energy in space and time, a short-pulse laser produces positrons more rapidly and in greater density than ever before in the laboratory. Chen's team is already preparing for ARC experiments that will leverage its high intensity for positron and electron–positron pair plasma research not possible elsewhere.

ARC's flexibility, precision, power, and unmatched ability to image dense materials will make it a valuable tool for exploring and advancing many of NIF's mission areas. When complete, ARC will be the highest energy short-pulse laser system in the world. Coupled with NIF, the highest energy long-pulse laser system, the duo will facilitate experiments and capture experimental details as never before. "The Laboratory previously achieved laser records for highest average and peak laser power, and now NIF has the record for highest energy," says John Heebner, an optical scientist on the ARC team. "Through these efforts, we are pushing the frontiers of what can be done with light."

—Rose Hansen

Key Words: Advanced Radiographic Capability (ARC), frequency-resolved optical gating, laser beam centering and pointing system, multilayer dielectric grating, petawatt laser, x-ray radiography.

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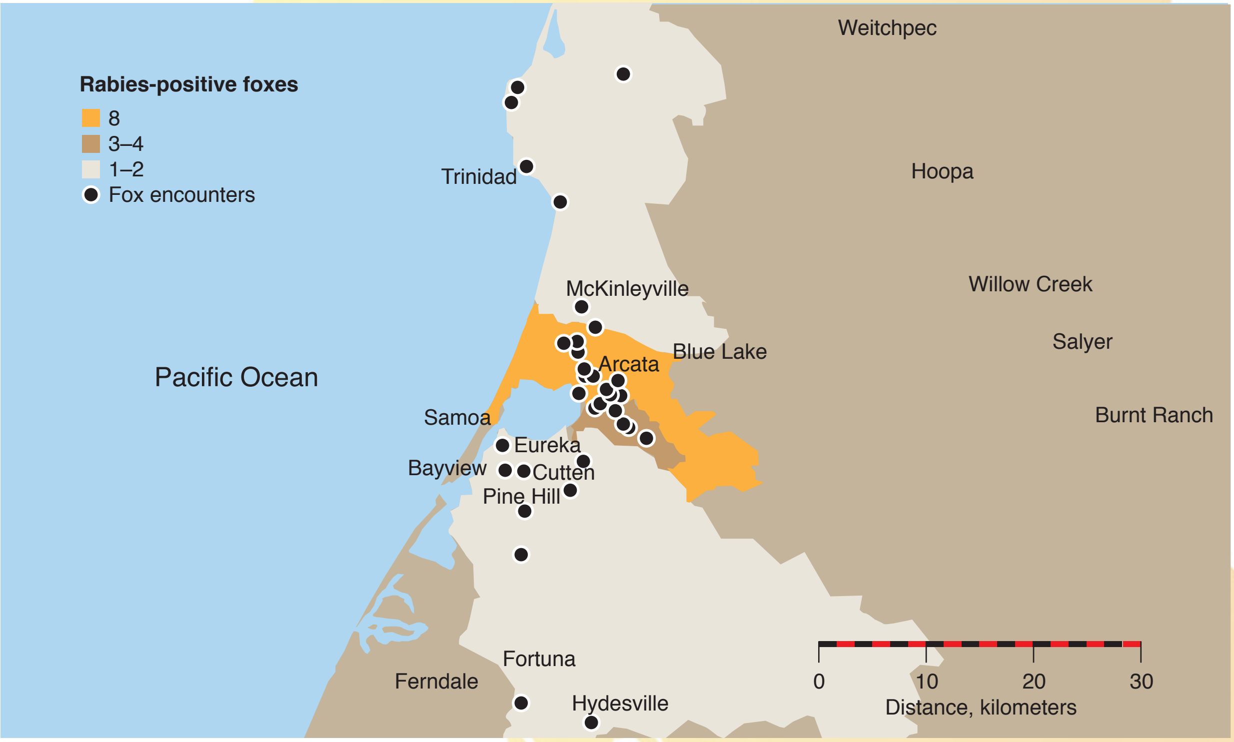
A New Method to Track Viral Evolution

IN 2009, Humboldt County in northwest California experienced an unusual rabies outbreak. Scientists at the California Department of Public Health observed a dramatic increase—up 355 percent—in the number of foxes with the virus. Rabies is a viral disease that affects the central nervous system and can be spread to humans through bites or scratches by rabid animals. Human rabies cases are exceedingly rare in the U.S., in large part because domestic animals are vaccinated against the disease. However, if preventive treatment is not administered to an infected person before symptoms develop, the disease is almost invariably fatal.

The typical rabies virus found in California terrestrial animals is the skunk variant, meaning skunks are the hosts that transmit it to other animals. Skunks with rabies tend not to attack people or other animals that share their habitat, but rabid foxes do, making the Humboldt County outbreak a concern for health officials.

Sharon Messenger, a virologist at the Department of Public Health, suspected that the 2009 outbreak was being spread through a phenomenon called species or host jumping. She asked a team of Livermore researchers, led by biomedical scientist Monica Borucki in the Physical and Life Sciences Directorate, to examine brain tissue samples collected from infected animals. The team, which includes Livermore scientists Jonathan Allen, Haiyin Chen, Tom Slezak, and Clinton Torres in the Computation Directorate, theorized that the rabies genes mutated as the virus jumped from skunks to foxes. The researchers are now using the Laboratory's computational resources and their expertise in bioinformatics to

In support of the California Department of Public Health, Livermore researchers analyzed samples of rabies genome taken from skunks and foxes using ultradeep sequence analysis.



A map of Humboldt County in California shows the fox encounters and rabies-positive foxes reported from January 1 through August 18, 2009.

better understand the evolution of rabies and other ribonucleic acid (RNA) viruses, an essential step toward improving biological defense against these diseases.

Going Viral

RNA viruses mutate about 1,000 times faster than bacteria and DNA-based viruses, and many of the new diseases infecting people are RNA viruses that have jumped from animal hosts. These diseases are a homeland security concern, particularly those that have pandemic or epidemic potential, and the Department of Defense considers viral infections a significant threat to soldiers deployed around the world.

The Livermore researchers are developing a more sensitive approach to identify mutations and predict which ones have the potential to jump from host to host. "We're interested in understanding how a virus population changes as it adapts from one host species to another," Borucki says. Initially supported by Livermore's Laboratory Directed Research and Development Program, the team's work is now funded by the Defense Threat Reduction Agency. Says Allen, "This study is giving us a new appreciation for the complexity and dynamism of viral evolution."

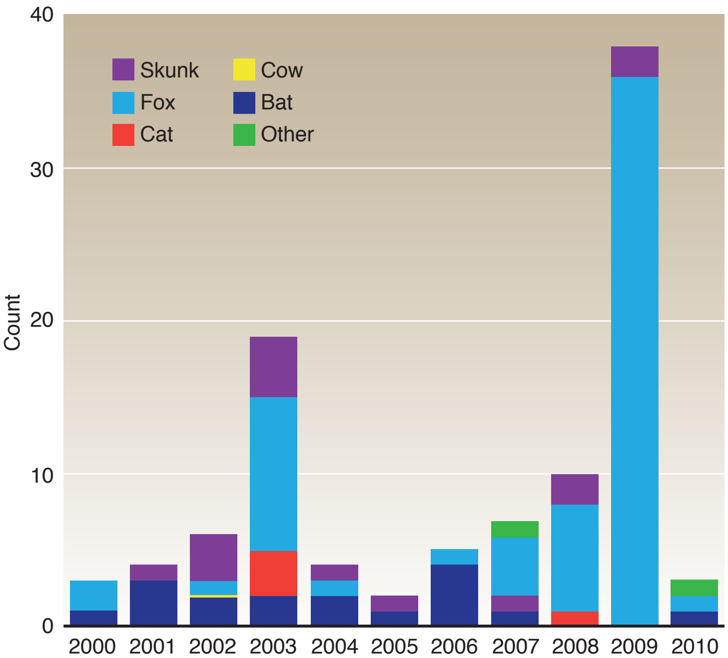
To understand how viruses mutate, the Livermore team is analyzing 50 rabies samples from the Humboldt outbreak as well as 35 samples of bovine coronavirus—another RNA virus—previously used in experiments to simulate a host-jumping event. In the exploratory stages, the researchers are developing computational tools that can analyze viruses to identify trends and potentially important mutations—what Allen calls "mutation prospecting." They will use this information to build a database that, when combined with viral studies at other laboratories, can help them spot rare variants and predict which viruses are most likely to jump from host to host.

Genetic variations found in terrestrial animals that carry rabies indicate each animal's geographic location. The rabies virus in a California skunk looks genetically different from that of a skunk in Texas. Thus, when a person contracts rabies, a small part of the viral sequence can be analyzed to determine its source, for example, as a raccoon variant from South Carolina.

"Although the rabies virus has jumped species multiple times in the past, it is still a relatively rare occurrence," says Borucki. "For example, a bat rabies virus in Arizona changed to infect skunks one year. Then nine years later, it changed to infect foxes." Genetic sequencing indicates that fox-to-fox transmission caused the Humboldt County outbreak. However, the virus originated in a skunk and jumped to a fox. According to Allen, the researchers' hypothesis is that mutations acquired by the virus allowed it to move through the fox population quickly.

Capturing Uncommon Variants

In working with the rabies virus, researchers normally sequence only a small part of its genome, about 300 to 400 nucleotides taken from up to 30 copies of the viral RNA. Genome sequencing technology generates copies from random fragments of a genetic sample, and researchers piece those snippets together to look for



This graph compares the number of rabies-positive animals in Humboldt County from 2000 to 2010.

patterns in the variants. The Livermore team uses a technique called ultradeep genome sequencing, which provides more coverage of a given population. In the Humboldt County study, the team analyzed 11,000 of the 12,000 total nucleotides in the rabies genome, using 300,000 copies of the genetic material. Such in-depth analysis provides a more complete picture of the rabies genome, including the uncommon variants in the virus, and helps clarify the diversity of the viral strains.

Some viruses evolve through recombination, a process in which genes swap information. Two viruses might even enter the same cell and take pieces from each other's genomes to create a new disease, such as the coronavirus mutation that led to severe acute respiratory syndrome. "In our work with the bovine coronavirus genome, we found samples with an extra piece of an amino acid sequence that appears to serve a biological function," says Borucki. "This piece commonly doesn't show up in surface analysis. We found the variant at a deeper level when we extended the population analysis." Uncovering such a variant is crucial because it could be the one that supports the mutation needed for a virus to infect another species.

The team is also experimenting with a method that is less deep but includes longer fragments. "Generally, we look at mutations in isolation, but they are most likely correlated with other parts of the genome," says Allen. "Two mutations might be in close proximity but not picked up on the same fragment. By reading a longer fragment, we could potentially establish that the two mutations link to the same gene."

Trending Data

The researchers plan to document all of the mutations and differences found in the sample genetic data. Both methods, ultradeep sequencing and long-fragment analysis, will yield huge amounts of data, which will require high-performance computing resources to analyze. Borucki says, "Without Livermore's biocomputational and mathematic capacity, we couldn't do this kind of experiment." Sequencing a single sample generates about 1.5 billion bytes of data in a compressed format. The team has already processed about 70 samples. A 300-sample study would require half a trillion bytes of storage capacity. The data files must also be professionally maintained and backed up, which requires Livermore's information technology expertise.

Allen is working on a software code to organize the data so researchers can discover trends. As sequencing technology gets faster and cheaper, real-time processing will be possible, allowing scientists to predict which viruses are likely to jump from host to host. Tools that can help them understand the potential function of virus changes and the variability present in a virus population could be a boon for forensic studies and vaccine development.

Borucki is also using results from this project to educate people about rabies. She notes that many people do not understand that it doesn't take a bite to be infected with rabies. The disease can be transmitted by a scratch from an infected feral cat, for example, and delays in treatment are dangerous. "When I talked to Livermore high school students, few of them knew that rabies is nearly 100 percent fatal in humans," Borucki says. "By getting this issue on people's radar, we have the potential to influence their behavior."

In the future, the Livermore analysis tools could be used to look for trends in viruses in different environmental situations. With a sufficient pool of candidate mutations—another piece of the data puzzle still needed—public health officials could identify new viral threats to humans in time to produce vaccines against those particular bugs. With advance warning, medical professionals and first responders could then treat the initial infections more efficiently and reduce the need for mass immunizations.

—Kris Fury

Key Words: bovine coronavirus, genetic variation, genome, host jumping, mutation, sequencing, rabies, ribonucleic acid (RNA) virus.

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Data for Defense
New Software Finds It Fast

LAWRENCE Livermore has a long history partnering with the Department of Defense (DoD) to help meet emerging national security needs. Over the past several decades, Livermore researchers have provided DoD agencies with both hardware and software solutions for enhanced missile defense, conventional weapons, armor and antiarmor materials and munitions, remote sensing, secure communications, sensors to detect weapons of mass destruction (WMD), and operational planning tools.

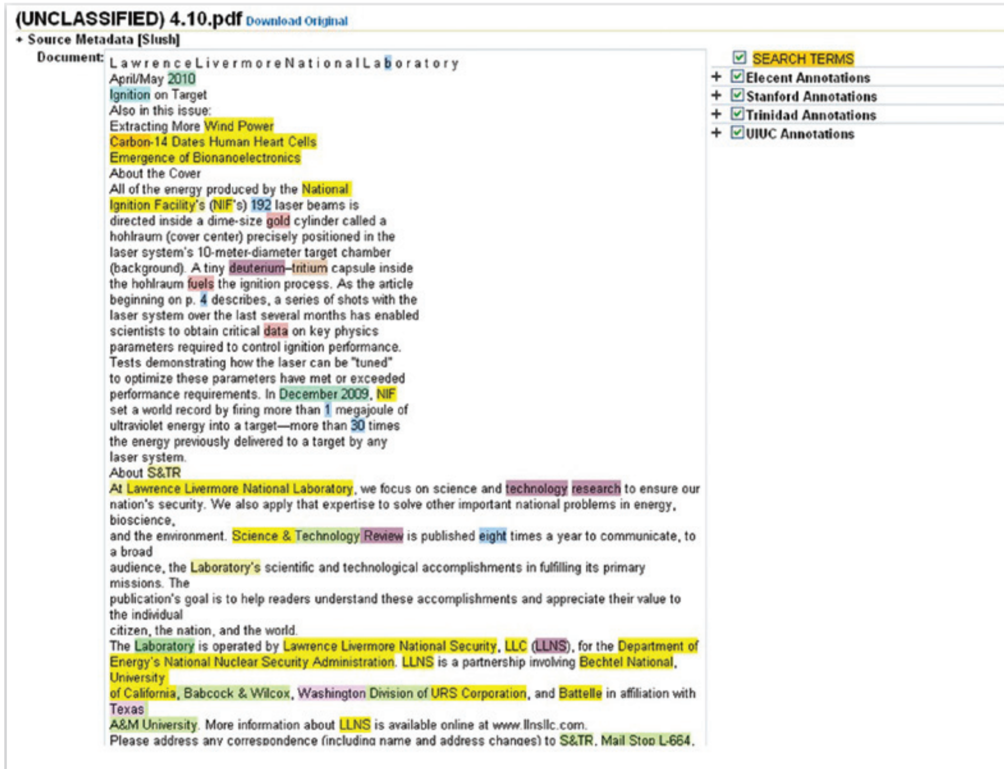
In fact, DoD investments continue to grow and now support multiple strategic science and technology areas at Livermore, further validating that the department is a key work sponsor and partner for the Laboratory. Dave Brown, program director for Defense in Livermore's Office of Strategic Outcomes, says, "My job is to understand the needs, requirements, and budgets of the Department of Defense and then determine within the Laboratory where we can provide technical solutions that leverage our science and technology expertise."

According to Brown, some of the products most valued by DoD have been developed by Livermore software experts to help warfighters and military planners distill, combine, relate, manipulate, and access massive amounts of data in a timely manner. Quickly isolating that information is a growing problem. Because of data overload, analysts typically spend more time collecting data than analyzing it.

Too Much Data, Not Enough Time

"Warfighters have way too much data to process in a timely manner," says Brown. "Sophisticated algorithms and other software can help them extract what they need to make decisions fast." For example, Livermore computer science and engineering experts developed Persistics, a data-processing pipeline that efficiently extracts pertinent information from enormous amounts of video data collected by unmanned aircraft. (See *S&TR*, April/May 2011, pp. 4–11.)

Another valuable resource is the Counterproliferation Analysis and Planning System (CAPS), an information system used by the U.S. Armed Forces to plan missions against facilities that support WMD production. In 1998, then Secretary of Defense William Cohen selected CAPS as the preferred planning tool to combat WMD. CAPS provides in-depth assessments of facilities,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April/May 2010
Ignition on Target
Also in this issue:
Extracting More Wind Power
Carbon-14 Dates Human Heart Cells
Emergence of Bionanoelectronics
About the Cover
All of the energy produced by the National
Ignition Facility's (NIF's) 192 laser beams is
directed inside a dime-size gold cylinder called a
hohlraum (cover center) precisely positioned in the
laser system's 10-meter-diameter target chamber
(background). A tiny deuterium–tritium capsule inside
the hohlraum fuels the ignition process. As the article
beginning on p. 4 describes, a series of shots with the
laser system over the last several months has enabled
scientists to obtain critical data on key physics
parameters required to control ignition performance.
Tests demonstrating how the laser can be "tuned"
to optimize these parameters have met or exceeded
performance requirements. In December 2009, NIF
set a world record by firing more than 1 megajoule of
ultraviolet energy into a target—more than 30 times
the energy previously delivered to a target by any
laser system.
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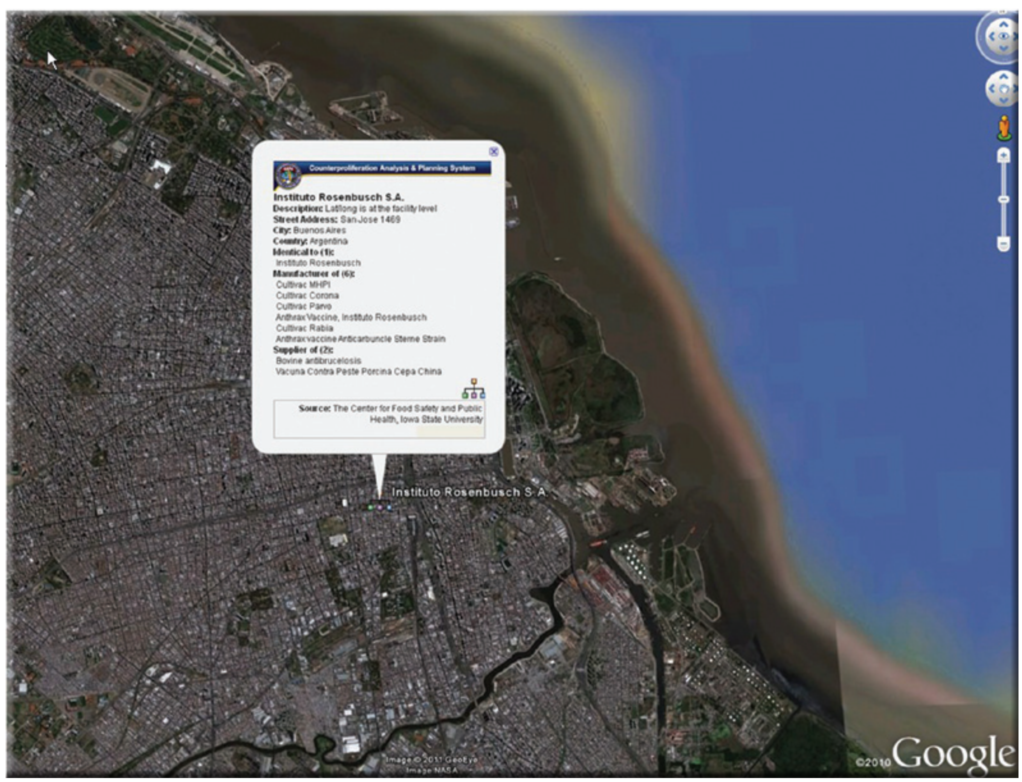
SEARCH TERMS
+ Elecent Annotations
+ Stanford Annotations
+ Trinidad Annotations
+ UIUC Annotations

With Trinidad, analysts can efficiently sift through vast amounts of information by zooming in on key terms and highlighting them. As an example, Trinidad analyzed text from a recent issue of *S&TR*. Color highlights indicate successful "hits" for different search terms.



The EleCent Earth application summarizes data in a geospatial display. Users search EleCent data by geographic area and topic of interest, and results are mapped with the Google Earth plug-in. Icons denote "hits" in the selected geographic area, and clicking on an icon produces summary information about that site. In this example, an EleCent search reveals a company in Buenos Aires that produces veterinary pharmacological products.

determines the potential for collateral damage from interdiction attempts, and quantifies the signatures that can reflect ongoing operations at selected sites.

Accessed through the major classified military networks, CAPS has supported several missions, including the Kosovo conflict, Operation Enduring Freedom, and Operation Iraqi Freedom, as well as relief efforts following catastrophic events such as earthquakes. The CAPS staff at Livermore also provides a daily technical reachback capability in response to requests from warfighters and planners.

Over the past few years, software developers have focused on making the vast amount of information residing in the CAPS data warehouse more manageable. CAPS stores more than 810 million documents, and billions of relationships link the data they contain. By designing an intuitive, easy-to-use computer interface for the system, the development team reduced data retrieval from hours to nearly real-time output, thereby freeing time for DoD personnel to perform in-depth analyses. In 2010, the team received a Global Security Silver Award for its success.

Two key components speed data extraction and enhance understanding. The first, Trinidad, provides a powerful data "triage" capability for quickly identifying pertinent high-value information while discarding the rest. Trinidad helps users more efficiently sift through mountains of unstructured data including open-source articles, scientific publications, Web-based news, and government reports—all of which contain information associated with a particular mission.

Trinidad leverages Hadoop, open-source software designed for reliable, scalable, and distributed computing, as well as the latest techniques for natural language processing. Advanced algorithms developed by Livermore researchers identify and zoom in on key terms or knowledge from subject-matter experts. A Web interface helps analysts with data triage by prioritizing documents and identifying items of interest. Search criteria can be a simple term or list of terms or complex phrases defined by Boolean relationships using the words *and*, *or*, and *not*. The resulting report highlights important terms so analysts can scan the relevant documents quickly. Trinidad can run on a laptop or a much more powerful Linux computer cluster.

The second component, Element Centric (EleCent), allows users to store, update, retrieve, and analyze data categorized as critical or related to a CAPS mission. EleCent combines an enormous database with Web-based tools for viewing results in various formats, from tabular lists to geospatial maps. EleCent uses Grails, an open-source application framework for rapidly developing Web-based tools. The data to be analyzed are derived from many sources, including commercial data sets and results from Livermore's defense-related research.

The EleCent Editor application allows authorized users to enter, edit, verify, and export data. The Editor serves as a tracking mechanism for every piece of data (element) in the system. Before information is entered into EleCent, a subject-matter expert at Livermore reviews it for accuracy. It then becomes available for external customers and is automatically included in the data triage performed by Trinidad. Users may then explore the relevant Trinidad documents identified by the Editor for a particular search element. In addition, filtering options allow users to easily find, select, and bin data and export those results to other tools for further analysis.

Providing a Geospatial View

Another tool designed by the Livermore team is EleCent Earth. This application uses the Google Earth plug-in to display results in a geospatial format as well as in a tabular list. With EleCent Earth, users can search by geographic area plus topic of interest. Results are plotted on a map at the level of detail selected by a user (either world, regional, or country view). Icons mark the "hits," or search results returned, for the specified area. Clicking on an icon produces a summary of the site, including its name, type, location, Web address, and other information.

In 2011, the CAPS team showcased the flexibility of the EleCent software architecture in a proof-of-concept demonstration for a potential sponsor. The sponsor's database was structured in such a way that made it difficult for other organizations to import and host. Livermore developers imported the data set into EleCent and processed it with the EleCent Editor. The data were immediately viewable by users, who could then sort, export, and exploit the information.

Trinidad and EleCent have received highly favorable reviews from DoD analysts worldwide. Together, the two components make CAPS an even more powerful tool for U.S. warfighters. "CAPS provides stellar, accurate knowledge in a format that can be readily analyzed so a warfighter can make sound decisions quickly," says Brown.

He notes that the Laboratory puts a lot of science behind every DoD product. "To the casual observer, CAPS may look like a simple Web browser, but we have many years of development effort behind it," says Brown. "Whether we're developing software, hardware, or a combination of both, our goal is to take technically complex problems and produce operationally relevant solutions for the warfighter."

—Arnie Heller

Key Words: Counterproliferation Analysis and Planning System (CAPS), Element Centric (EleCent) component, Google Earth, Grails application, Hadoop software, Trinidad component, weapons of mass destruction (WMD).

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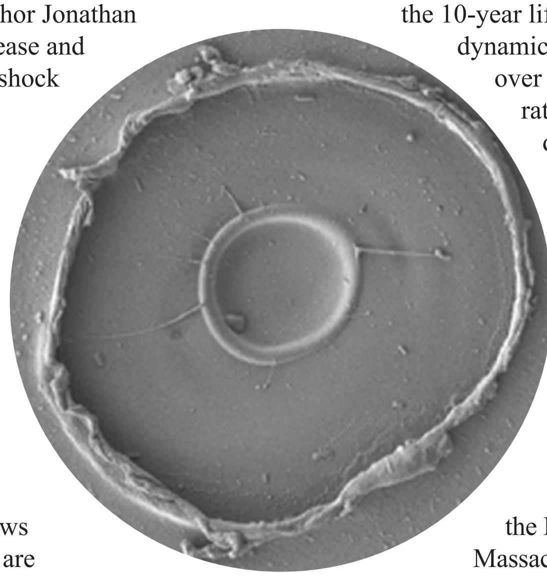
The Laboratory in the News (*continued from p. 2*)

Compression Experiments Yield Shocking Results

Using an ultrafast spectroscopic technique, a team of Livermore scientists measured breakouts in aluminum thin films undergoing laser-induced shocks at accelerations of up to 10 trillion g—1 trillion times faster than a jet fighter in a maximum turn. In about 20-trillionths of a second, pressure on the samples reached 40 gigapascals, allowing the researchers to observe how an aluminum sample (shown below) responds to dynamic compression at ultrahigh strain rates. Results from the team's research appeared in the September 30, 2011, issue of *Physical Review Letters*.

Controlled shock compression has been used for decades to examine the behavior of materials under extreme pressures and temperatures. However, scientists have not previously observed the microscopic details of solid materials undergoing rapid deformation. "In solids, a sufficiently large amplitude shock produces irreversible plastic deformation and relaxes the initial stress," says Livermore physicist and lead author Jonathan Crowhurst. If the amplitude continues to increase and the shock drive is maintained, a steady-wave shock profile evolves. Results from the experiments indicate that the wavefront will propagate indefinitely without a change in the profile form.



According to coauthor Michael Armstrong, the team's original goal was to demonstrate that measurements acquired on ultrafast timescales were consistent with those from longer experiments. In achieving that goal, he says, "We got a surprise—unexpected insight into shock-wave phenomena." As a result, experiments can for the first time test fundamental scaling laws on time and length scales where those laws might begin to break down at strain rates that are orders of magnitude larger than previously examined.

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Variations Found in Fat Removal Rates

Results from an international collaboration involving Livermore scientist Bruce Buchholz indicate that fat "turnover" rates are significantly slower in obese people than they are in people of average weight, and this rate differential arises from the different rates at which triglycerides are stored in and removed from fat cells. "In our study, we found a slower output of fat in obese people," Buchholz says. As a result, the fat stored in obese individuals is 2 years old on average compared with 1.5 years for people within the normal weight range.

Using accelerator mass spectrometry (AMS), the team measured carbon-14 ratios in lipocytes (human fat cells) within subcutaneous adipose tissue, the major fat depot for humans. Carbon dating is a common approach in archaeology and paleontology to determine the age of artifacts. In the fat-cell study, the team applied the technique to analyze the age of fat and how fast it turns over in humans.

AMS measurements showed that fat is replaced six times during the 10-year lifespan of the average fat cell, enabling a dynamic regulation of fat storage and movement over time. In obese individuals, however, the rate at which fat is removed from fat tissue decreases, and the amount of fat stored each year increases. In contrast, fat storage and removal rates balance in non-obese people for no net increase in fat. Results from this study appeared in the October 6, 2011, issue of *Nature*.

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A New Era of Plasma Nuclear Science

Researchers from Lawrence Livermore, the Plasma Science and Fusion Center at the Massachusetts Institute of Technology, and the Laboratory for Laser Energetics at the University of Rochester used the OMEGA laser at Rochester to precisely measure a fundamental nuclear process—the elastic scattering of neutrons off heavy forms of hydrogen. This experiment marks the first time a fundamental nuclear physics cross section was measured with a high-energy-density laser instead of a conventional accelerator.

In the experiment, OMEGA's 60 laser beams strike the outer surface of a glass capsule only 1 millimeter in diameter and filled with deuterium and tritium, the heavy isotopes of hydrogen. The laser beams generate a hot, dense plasma, in which electrons are stripped from their parent atoms to create an interpenetrating gas, or "soup," of positive and negative charges on the capsule's surface. The rapidly expanding plasma gas causes the capsule to implode, creating an extremely hot (100-million-kelvin) plasma of deuterium–tritium ions and electrons.

A small fraction of these ions fuse together, a process that generates a neutron traveling at one-sixth the speed of light with about 14.1 million electronvolts of energy. In contrast, an ordinary chemical reaction, such as the burning of wood or coal, produces just 1 electronvolt of energy. As the energetic neutrons race out of the imploding capsule, a small fraction collides and scatters, like billiard balls, off the surrounding deuterium–tritium ions.

The research team used these rare collisions and the corresponding transfer of energy from neutrons to ions to accurately measure the nuclear collision process. The team's results, which were published in the September 16, 2011, issue of *Physical Review Letters*, match theoretical calculations, providing evidence in support of nuclear theory. The reaction data produced in the experiments are also important for nuclear astrophysics and fusion energy research.

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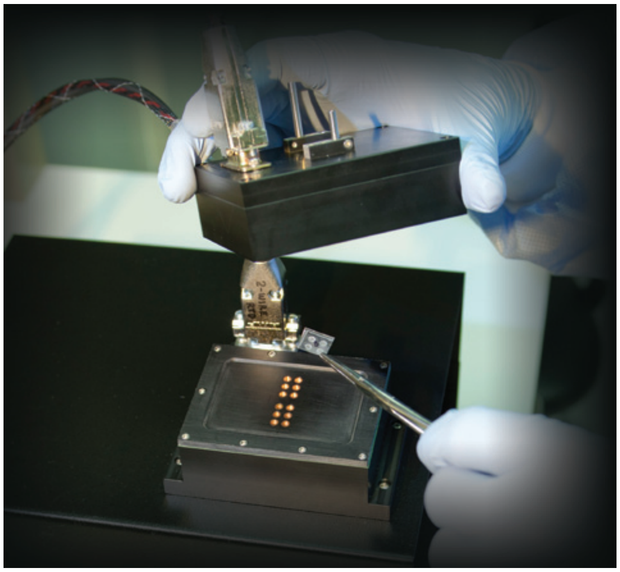

Diagnostic Device Analyzes DNA in Minutes

A Laboratory team led by engineer Reginald Beer has developed a new diagnostic technique that uses polymerase chain reaction (PCR) to amplify nucleic acids (DNA and RNA) and analyze samples in less than three minutes. The new device (left) reduces an hourlong process to mere minutes and has the potential to make PCR viable for medical point-of-care applications, emergency response, or widespread environmental monitoring.

PCR is an indispensable technique in medical and biological research laboratories worldwide. It allows researchers and clinicians to replicate a single piece of DNA or RNA millions of times. They can then use those copies for genome sequencing, gene analysis, inheritable disease diagnosis, paternity testing, forensic identification, and infectious disease detection.

The new device combines a porous material and a thin-film resistive heater to provide heating and cooling rates of 45°C per second and thermal cycling at speeds of less than 2.5 seconds. As a result, says Beer, "Our device cools as fast as it heats."

To test the technique, the Livermore researchers amplified genomic DNA from an *Enterobacter* bacterium, proving that the device could rapidly amplify a large DNA segment. This experiment demonstrated 30-cycle (billionfold) PCR amplification of the target DNA in 2 minutes and 18 seconds. A second test analyzed a sample of severe acute respiratory syndrome to show the device's utility in handling a public health threat virus. The team's report, which was published in the July 27, 2011, issue of *Analyst*, was the journal's most-accessed article for August 2011.

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In this section, we list recent patents issued to and awards received by Laboratory employees. Our goal is to showcase the distinguished scientific and technical achievements of our employees as well as to indicate the scale and scope of the work done at the Laboratory.

Patents

Hazardous Particle Binder, Coagulant and Re-Aerosolization Inhibitor

Paula Krauter, David Zalk, D. Mark Hoffman
U.S. Patent 7,922,644 B2
April 12, 2011
This copolymer and water–ethanol solvent solution can bind with airborne contaminants or potential airborne contaminants, such as biological weapon agents or toxic particulates. As the solvent evaporates, coagulation causes the contaminants to adhere to a surface, which inhibits their resuspension. The solution uses a water or ethanol–water mixture for the solvent and a copolymer with one of several functional group sets so as to have the physical and chemical characteristics of high adhesion, low viscosity, low surface tension, negative electrostatic charge, substantially neutral pH, and a low dissociation constant (pKa). Use of the copolymer solution prevents the reaerosolization and transport of unwanted, reactive species, thus increasing health and safety for personnel charged with decontaminating buildings and areas.

Dichroic Beamsplitter for High Energy Laser Diagnostics

Kai N. LaFortune, Randall Hurd, Scott N. Fochs, Mark D. Rotter, Lloyd Hackel
U.S. Patent 8,009,283 B2
August 30, 2011
Wavefront control techniques are provided for the alignment and performance optimization of optical devices. A Shack–Hartmann wavefront sensor measures the wavefront distortion. A control system then generates a feedback error signal and sends it to the optics inside the device to correct the wavefront. The system can be calibrated with a low-average-power probe laser. The optical device is coupled to a diagnostic and control package in a way that optimizes the device's output power and the coupling of the probe light into the diagnostics.

Awards

Bruce Remington, group leader for material dynamics in the National Ignition Facility and Photon Science Principal Directorate, received the **2011 Edward Teller Medal** from the **American Nuclear Society Fusion Energy Division**. Remington was cited for his "pioneering scientific work in the fields of inertial confinement fusion, laboratory astrophysics and high pressure material science and leadership in development of an international effort in high energy density laboratory astrophysics."

Remington joined the Laboratory in 1988 as a physicist in the Inertial Confinement Fusion (ICF) Program, where he pioneered the use of lasers to study matter under extremely high pressure. He has led experiments in ICF implosion physics, hydrodynamic instabilities, ablation-front dynamics, radiative hydrodynamics, turbulent hydrodynamics, laboratory astrophysics, and solid-state material dynamics.

The Edward Teller Medal recognizes pioneering research and leadership in the use of lasers, ion-particle beams, or other high-intensity drivers to produce unique high-density matter for scientific research and to conduct investigations of inertial fusion. Established in 1991, the medal honors the late Edward Teller, a former Laboratory director who was recognized worldwide as a pioneer in inertial fusion science.

Lawrence Livermore selected **Madhav Marathe** as the inaugural **George A. Michael Distinguished Scholar**. This annual award honors the memory of Livermore physicist and computational scientist George Michael, who was an early pioneer of the field now known as supercomputing and helped found the annual Supercomputing Conference. The scholarship offers a noted scientist the opportunity to conduct research at the Institute for Scientific Computing Research, which fosters collaborations between Livermore and academic researchers in the areas of scientific computing, computer science, computational mathematics, and other topics in support of Laboratory missions.

Marathe is a professor of computer science and deputy director of the Network Dynamics and Simulation Science Laboratory for the Virginia Bioinformatics Institute at Virginia Tech in Blacksburg, Virginia. He is a recognized expert in interaction-based modeling and in simulating complex biological, information, social, and technical systems.

Livermore computer scientist **Greg Bronevetsky** is one of 94 recipients of the **Presidential Early Career Award for Scientists and Engineers**, the highest honor bestowed by the U.S. government on science and engineering professionals in the early stages of their independent research careers. Bronevetsky, who works at the Center for Applied Scientific Computing, was selected for helping advance the state of the art in high-performance computing. His research focuses on ensuring that the increasing power, size, and complexity of supercomputers do not come at the expense of reliability. The methodologies he is developing allow researchers to study how hardware failures on machines with millions of components are likely to influence the design of next-generation high-performance computers and the software applications that run on them.

Abstract

Simulating the Next Generation of Energy Technologies

The energy and environmental challenges facing the nation are immense and urgent, and high-performance computing (HPC) promises to be an important tool for accelerating the development and deployment of solutions. Lawrence Livermore is pursuing a number of HPC projects to better understand the intricacies of clean-energy use and generation. Simulations are helping researchers gain insights into new technologies and estimate the performance of systems too complex for conventional analysis. The Laboratory's HPC resources provide the computational horsepower needed to illustrate complex scenarios in detail so utility companies and resource developers can evaluate the viable options. These projects are demonstrating the competitive advantage HPC offers to help the nation solve environmental challenges and achieve energy independence, reducing its reliance on imported fossil fuels. Using HPC tools to explore technology solutions will also save time and money by helping utility companies reduce capital expenditures, avoid industrial failures, and prevent damage to power-generation equipment.

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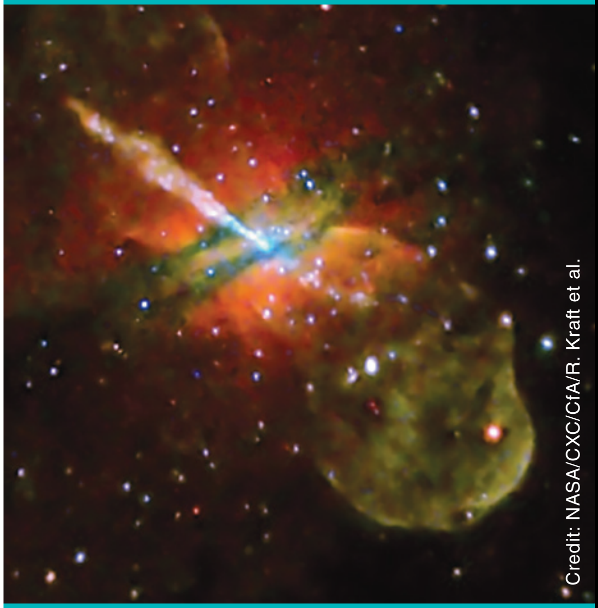
Coming Next Issue

Science on NIF



Credit: NASA/CXC/CfA/R. Kraft et al.

The National Ignition Facility enables researchers to explore the formation and evolution of stars and planets.

Also in January/February

• The Laboratory's expertise in radionuclide analysis and atmospheric dispersion modeling contributed to the nation's support for Japan following the 2011 earthquake and nuclear accident.

• The Web-based MIDAS program is a valuable resource for experiments and simulations involving materials for stockpile stewardship and other national security programs.

• A novel computer architecture based on "persistent" memory eases data-intensive computations to find a single anomalous bit out of a billion.

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